

Curriculum Vitae of Dmitry I. Lyakh (Liakh), Ph.D.

R&D Scientist, Scientific Computing
National Center for Computational Sciences
Oak Ridge National Laboratory
Oak Ridge, TN 37831

E-Mail: liakhdi@ornl.gov
E-Mail: quant4me@gmail.com
Phone: +1(865)574-7783
Skype: **DmitryLyakh**

PROFESSIONAL EXPERIENCE

- **Computational Scientist** (high-performance computing). National Center for Computational Sciences, Oak Ridge National Laboratory, Oak Ridge, TN: Sep 2014 – active.
- Post Doctorate Associate. National Center for Computational Sciences, Oak Ridge National Laboratory (supervisor: Dr. T. Straatsma): Dec 2013 – Aug 2014.
- Adjunct Post Doctorate Associate. Research Group of Prof. Rodney J. Bartlett, Quantum Theory Project, University of Florida, Gainesville, FL, USA: “Development and massively parallel implementation of accurate methods for electronic structure calculations”: Jun 2009 – Dec 2013.
- Researcher. Astrochemistry group, School of Chemistry, V.N. Karazin Kharkiv National University, Kharkiv, Ukraine: Jul 2008 – May 2009.
- Lecturer. School of Chemistry, V.N. Karazin Kharkiv National University, Kharkiv, Ukraine. Courses: Quantum Chemistry and Quantum Mechanics, Linear Algebra and Computer Programming for chemists: Sep 2008 – May 2009.

EDUCATION

- **PhD in Chemistry** (Physical Chemistry: Computational Chemistry & Cheminformatics). School of Chemistry, Karazin Kharkiv National University, Kharkiv, Ukraine: Nov 2005 – Feb 2009. (Thesis: “*The coupled cluster theory in ab initio calculations of potential energy surfaces of small molecules*”; advisor Prof. V. V. Ivanov). Defended with honors on Feb 19, 2009.
- MS Degree with honors (Quantum chemistry and Cheminformatics). School of Chemistry, Karazin Kharkiv National University, Kharkiv, Ukraine: Sep 2004 – Jul 2005. (Thesis: “*An index based approach for describing electron correlation effects in the coupled cluster theory*”).
- BS Degree with honors (Quantum Chemistry and Cheminformatics). School of Chemistry, Karazin Kharkiv National University, Kharkiv, Ukraine: Sep 2000 – Jul 2004. (Thesis: “*The coupled cluster theory with an explicit account of higher excitations*”).

SPECIALIZED AREAS OF KNOWLEDGE AND EXPERTISE

- Method and algorithm development for high-performance heterogeneous computing;
- Computational and quantum chemistry; Electronic structure theory;
- Quantum many-body problem, coupled-cluster theory, tensor network state theory;
- Computer programming in modern Fortran (2003+), C/C++, Assembler, Python;
- Parallel programming with MPI, OpenMP, CUDA, OpenACC, MIC directives;
- Development of software libraries for numerical tensor algebra;
- Development of software tools for simulating quantum computing circuits;
- Development of software tools for automated symbolic tensor algebra manipulations;
- Development and use of domain-specific computer languages and corresponding runtimes for massively parallel computations in the field of quantum many-body theory;
- Some experience with QSAR (Quantitative Structure-Activity Relationship) and ComFA (Comparative Field Analysis).

PUBLICATIONS

29 articles in peer-reviewed journals (attached), **3 book chapters**, more than 20 presentations, more than **600 citations**; ***h-index* 13**.

Curriculum Vitae of Dmitry I. Lyakh (Liakh), Ph.D.

AWARDS AND GRANTS OF PRINCIPAL PARTICIPATION

- Internal ORNL grant “Enabling Quantum Acceleration in Scientific High Performance Computing”, PI A. J. McCaskey, Oct 2016 – Sep 2018.
- Grant of the Air Force Office for Scientific Research (AFOSR), STTR#AF09-BT40, Grant# F09B-T40-0149, Phase II, “Coupled-cluster methods for multi-reference applications”, PI Prof. R. J. Bartlett, Jun 2011 – May 2012.
- Grant of the Air Force Office for Scientific Research (AFOSR), STTR#AF09-BT40, Grant# F09B-T40-0149, Phase I, “Coupled-cluster methods for multi-reference applications”, PI Prof. R. J. Bartlett, Jun 2010 – Feb 2011.
- Grant of the Kharkiv National University Foundation for applied and fundamental research, Grant#10-09, “Efficient computer-aided techniques for identification and predicting the bioactivity of complex organic molecules”, PI Prof. V. Ivanov, Jan 2009 – Dec 2009.
- Travel grant of the US Department of Energy for attending the International Program “Atomic, Chemical, and Nuclear Developments in Coupled Cluster methods”, Institute for Nuclear Physics, University of Washington, Seattle, WA, USA, Jun 23 – Jul 25, 2008.
- Grant of the National Foundation for Fundamental Research (Ukraine) „Influence of the electron correlation effects on magnetic and electric properties of non-carbon built nano-materials”, PI Prof. V. O. Cheranovskii, 2007-2009 years.
- An honorary scholarship established in memory of Prof. I. Tarapov, V. N. Karazin Kharkiv National University, 2006-2007 academic year.
- Grant of the Kharkiv National University Foundation for applied and fundamental research, Grant#17-05 “Informational technologies and computer-aided methods for predicting activity of chemical substances”, PI Prof. V. O. Cheranovskii, 2004-2005 academic year.
- Travel grant from INTAS for attending the V. A. Fock International Conference in Quantum Chemistry, Velikiy Novgorod, Russia, May 3-10, 2005.
- An honorary scholarship by the Yu. Sapronov charitable organization, 2004-2005 academic year.
- The Kharkiv Mayor honorary scholarship, 2003-2004 academic year.
- First award at the 4th Ukrainian conference for graduate and undergraduate students “Contemporary problems of chemistry”, Kyiv, Ukraine, May 21-22, 2003.

SOFTWARE DEVELOPMENT

- **DIRAC** (contributor): US DOE Office of Science partly sponsored project (the CAAR program at the Oak Ridge Leadership Computing Facility): Work on the scalable accelerator-enabled infrastructure for large-scale tensor algebra for relativistic coupled-cluster theory (large-scale relativistic electronic structure simulations).
DIRAC code website: <http://diracprogram.org/doku.php>
DIRAC code statistics: Hundreds of license holders all over the world.
- **LS-DALTON** (contributor): OLCF CAAR program: Work on the distributed tensor algebra library that can support accelerators in order to enable the largest-scale electronic structure simulations based on the coupled-cluster theory.
LS-DALTON code website: <http://www.daltonprogram.org/>
- **NWChem** (contributor): OLCF CAAR program: Deployment of my tensor algebra library TAL-SH in the CCSD code for better utilization of NVIDIA GPU and multi-core CPU.
NWChem code website: http://www.nwchem-sw.org/index.php/Main_Page
NWChem code statistics: More than 60000 downloads from all over the world.
- **TAL-SH** (sole author): Basic tensor algebra library for shared-memory computing units (multi-core CPU, NVIDIA GPU, Intel Xeon Phi). Work in progress on deploying TAL-SH in NWChem, ACES III, DIRAC, and LS-DALTON software packages.
TAL-SH code website: https://github.com/DmitryLyakh/TAL_SH
- **cuTT** (contributor): Fast tensor transpose library for NVIDIA GPU.
cuTT code website: <https://github.com/ap-hynninen/cutt>
- **XACC** (contributor): Software infrastructure for hybrid quantum-classical HPC programming.
XACC code website: <https://github.com/ORNL-QCI/xacc>
- **Generic Fortran Containers, GFC** (sole author): Implementation of generic heterogeneous containers in modern Fortran-2003, including vector, linked list, tree, dictionary, graph, etc., capable of storing objects of any type/class

Curriculum Vitae of Dmitry I. Lyakh (Liakh), Ph.D.

in the same container.

GFC code website: <https://gitlab.com/DmitryLyakh/GFC>

- **ExaTENSOR** (sole author, under development): Massively parallel tensor algebra processor (virtual machine) for large-scale heterogeneous HPC systems: Given a list of human-readable formal tensor expressions, for example those associated with some quantum many-body method, ExaTENSOR translates this formal (domain-specific) language into an internal representation and executes (in real time) the corresponding machine-independent instructions on all physical computing units (CPU, GPU, MIC) available on the HPC system.
- **DiaGen** (sole author): Computer program for an automated (parallel) implementation of quantum many-body methods, with a particular emphasis on higher-order approaches (generation of higher-rank tensor equations, their spin-integration, factorization and cost reduction, translation into the target code).
- **ACESIII/IV** (contributor): Implementation of the tensor algebra library for multicore CPU and NVIDIA GPU in order to enhance efficiency on large-scale HPC systems. General design of massively parallel higher-rank tensor algebra.
ACES code website: <http://www.qtp.ufl.edu/aces/>
ACES code statistics: Hundreds of downloads.
- **Cluster** (sole author): Automated parallel (MPI) code implementing single- and multireference higher-rank coupled-cluster theory, based on the direct machine interpretation of the coupled-cluster equations (part of my PhD project).
- **Chromo** (sole author): Specialized computer program for the classification of chromatographic peaks in pharmaceutical research (side project).
- **BioSurf** (principal contributor): Computer program for building structure-activity relationships based on molecular fields as principal descriptors (side project).

SYNERGISTIC ACTIVITIES

- Member of the Editorial Board of the Journal of Quantum Chemistry (Hindawi), 2014-2016.
- Scientific journal referee: Journal of Chemical Theory and Computation, International Journal of Quantum Chemistry, Computer Physics Communications, Journal of Chemical Physics, ACM Transaction on Mathematical Software, WIREs Computational Molecular Science, Journal of Basic and Applied Physics.
- ALCF Theta Early Science Program proposal reviewer (Argonne Leadership Computing Facility (ALCF), Argonne National Laboratory).
- Invited participant of the US DOE Basic Energy Science (BES) Exascale Requirements gathering in Rockville, MD (Nov 2015): Delivering a roadmap to efficient Exascale computing for Basic Energy Sciences.
- OLCF INCITE proposal reviewer (Oak Ridge Leadership Computing Facility (OLCF) Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program, Office of Science, US Department of Energy).
- OLCF CAAR proposal reviewer (OLCF Center for Accelerated Application Readiness (CAAR) program, Office of Science, US Department of Energy).
- OLCF Director's Discretionary proposal reviewer (Oak Ridge National Laboratory).

COLLABORATIONS WITH OTHER SCIENTIFIC INSTITUTIONS

- Ohio State University, Columbus, OH, USA, group of Prof. Sadayappan (Computer Science department): Collaboration in the area of an efficient massively parallel implementation of quantum-chemistry codes on HPC systems: 02/2013 – 05/2013.
- University of Washington, Seattle, WA, USA, International Program at the Institute for Nuclear Theory devoted to the development of coupled-cluster methods for open-shell many-body systems: 04/01-04/13, 2013, supported by DOE.
- University of Washington, Seattle, WA, USA, International Program at the Institute for Nuclear Theory “Atomic, Chemical, and Nuclear Developments in Coupled Cluster methods”: 06/23 – 07/25, 2008, supported by DOE.
- University of Pisa, Pisa, Italy, group of Prof. B. Mennucci: Three weeks visit: 07/08/2007 – 07/29/2007, supported by NSF (USA).
- University of Arizona, Tucson, AZ, USA, group of Prof. L. Adamowicz:
 1. Three-month exchange program: 12/18/2006 – 03/19/2007, supported by NSF;
 2. Three-month exchange program: 03/29/2006 – 06/29/2006, supported by NSF.

Curriculum Vitae of Dmitry I. Lyakh (Liakh), Ph.D.

REFERENCES

- Dr. T. P. Straatsma. National Center for Computational Sciences, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA. E-mail: straatsmatp@ornl.gov
- Prof. Rodney J. Bartlett, Quantum Theory Project, University of Florida, New Physics Bldg #92, 2001 Museum Rd, Gainesville, FL, 32611, USA. Phone: +1(352)392-6974. E-mail: bartlett@qtp.ufl.edu
- Prof. Vladimir V. Ivanov, Chemistry, V.N. Karazin Kharkiv National University, 4 Sq. Svobody, Kharkiv, 61077, Ukraine. Phone: +38(057)707-5143. E-mail: vivanov@karazin.ua
- Prof. Ludwik Adamowicz, Dept. of Chemistry and Biochemistry, University of Arizona, 1306 E University Blvd, Tucson, AZ, 85721-0041, USA. Phone: +1(520)621-6607. E-mail: ludwik@email.arizona.edu

LIST OF PUBLICATIONS

PEER-REVIEWED ARTICLES (most recent first)

1. D. I. Lyakh. Efficient Electronic Structure Theory via Hierarchical Scale-Adaptive Coupled-Cluster Formalism: I. Theory and Computational Complexity Analysis // *Mol. Phys.*, -2017, *accepted*.
2. A.-P. Hynninen, D. I. Lyakh. cuTT: A High-Performance Tensor Transpose Library for CUDA Compatible GPUs // *ACM Transactions on Mathematical Software*, -2017, *submitted*.
3. B. A. Sanders, J. N. Byrd, N. Jindal, V. F. Lotrich, D. I. Lyakh, A. Perera, R. J. Bartlett. Aces4: A Platform for Computational Chemistry Calculations with Extremely Large Block-Sparse Arrays // *Proceedings of Parallel and Distributed Processing Symposium (IPDPS) 2017 IEEE International*, ISSN: 1530-2075, DOI: <https://doi.org/10.1109/IPDPS.2017.108>.
4. P. Baudin, D. Bykov, D. I. Liakh, P. Ettenhuber, K. Kristensen. A local framework for calculating coupled cluster singles and doubles excitation energies (LoFEx-CCSD) // *Mol. Phys.* -2017. DOI: <http://dx.doi.org/10.1080/00268976.2017.1290836>
5. T. Kjaergaard, P. Baudin, D. Bykov, J. J. Eriksen, P. Ettenhuber, K. Kristensen, J. Larkin, D. I. Liakh, F. L. Pawlowski, A. D. Vose, Y.-M. Wang, P. Jorgensen. Massively Parallel and Linear-Scaling Algorithm for Second-Order Møller-Plesset Perturbation Theory Applied to the Study of Supramolecular Wires // *Comp. Phys. Commun.* -2017. -V. 212. -P. 152-160.
6. I. A. Zaporozhets, V. V. Ivanov, D. I. Lyakh, L. Adamowicz. Discontinuities-free complete-active-space state-specific multi-reference coupled cluster theory for describing bond stretching and dissociation // *J. Chem. Phys.* -2015. -V. 143. -ID: 024109.
7. D. I. Lyakh. An efficient tensor transpose algorithm for multicore CPU, Intel Xeon Phi, and NVidia Tesla GPU // *Comp. Phys. Commun.* -2015. -V. 189. -P. 84.
8. D. I. Lyakh. Scale-adaptive tensor algebra for local many-body methods of electronic structure theory // *Int. J. Quantum Chem.* -2014. -V. 114. -P. 1607.
9. D. I. Lyakh, R. J. Bartlett. Algebraic connectivity analysis in molecular electronic structure theory II: Total exponential formulation of second-quantized correlated methods // *Mol. Phys.* -2014. -V. 112. -P. 213.
10. M. Musial, K. Kowalska-Szojda, D. I. Lyakh, R. J. Bartlett. Potential energy curves via double electron-attachment calculations: Dissociation of alkali metal dimers // *J. Chem. Phys.* -2013. -V. 138. -ID: 194103.
11. M. Musial, M. Olszowka, D. I. Lyakh, R. J. Bartlett. The equation-of-motion coupled cluster method for triple electron attached states // *J. Chem. Phys.* -2012. -V. 137. -ID: 174102.
12. D. I. Lyakh, R. J. Bartlett. A remark on the disconnected nature of Lagrange equations in the context of a linear-scaling implementation of the coupled-cluster energy gradients // *Mol. Phys.* -2012. -V.110. -P. 2343. (DOI:10.1080/00268976.2012.679639).
13. D. I. Lyakh. Algebraic connectivity analysis in molecular electronic structure theory I: Coulomb potential, tensor connectivity, ϵ -approximation // *Mol. Phys.* -2012. -V. 110. -P. 1469 (DOI:10.1080/00268976.2012.663509).
14. D. I. Lyakh, M. Musial, V. F. Lotrich, and R. J. Bartlett. Multireference nature of chemistry: The coupled-cluster view // *Chem. Rev.* -2012. -V. 112. -P. 182.
15. Vladimir V. Ivanov, Dmitry I. Lyakh, and L. Adamowicz. State-specific multireference coupled-cluster theory of molecular electronic excited states // *Annu. Rep. Prog. Chem. C.* -2011. DOI: 10.1039/c1pc90007b.
16. Dmitry I. Lyakh, Victor F. Lotrich, and Rodney J. Bartlett. The 'tailored' CCSD(T) description of the automerization of cyclobutadiene // *Chem. Phys. Lett.* -2011. -V. 501. -P. 166.
17. Dmitry I. Lyakh and Rodney J. Bartlett. An adaptive coupled-cluster theory: @CC approach // *J. Chem. Phys.* -2010. -V. 133. -ID: 244112.

Curriculum Vitae of Dmitry I. Lyakh (Liakh), Ph.D.

18. T. A. Klimenko, V. V. Ivanov, D. I. Lyakh, and L. Adamowicz. A calculation of spectroscopic parameters for hydrogen fluoride with multi-reference state-specific coupled-cluster method // *Chem. Phys. Lett.* – 2010. – V. 493. – P. 173-178.
19. T. O. Klimenko, V. V. Ivanov, and D. I. Lyakh. Potential energy surfaces of the ground and excited states of ^{11}BH molecule in the multireference coupled cluster theory // *Ukr. Phys. J. ISSN 2071-0194.* – 2010. – V. 55. – P. 657-664.
20. Vladimir V. Ivanov, Dmitry I. Lyakh, Ludwik Adamowicz. Multireference state-specific coupled-cluster methods. State-of-the-art and perspectives // *Phys. Chem. Chem. Phys.* – 2009. – V. 11. – P. 2355- 2370 (invited article).
21. D. I. Lyakh, V. V. Ivanov, L. Adamowicz. A generalization of the state-specific complete-active-space coupled-cluster method for calculating electronic excited states. // *J. Chem. Phys.* – 2008. – V. 128. – ID: 074101. – P. 1-15.
22. D. I. Lyakh, V. V. Ivanov, L. Adamowicz. State-specific multireference complete-active-space coupled-cluster approach versus other quantum chemical methods: dissociation of the N_2 molecule // *Mol. Phys.* – 2007. – V. 105. – No. 10. – P. 1335-1357.
23. V. V. Ivanov, L. Adamowicz, and D. I. Lyakh. Excited states in the multi-reference state-specific coupled-cluster theory with the CAS reference // *J. Chem. Phys.* – 2006. – V. 124. – No. 18. – ID: 184302 (9 pages).
24. D. I. Lyakh, V. V. Ivanov, and L. Adamowicz. Multireference state-specific coupled cluster approach with the CAS reference: inserting Be into H_2 // *Theor. Chem. Acc.* – 2006. – V. 116. –P. 427-433.
25. V. V. Ivanov, L. Adamowicz, and D. I. Lyakh. Potential energy surface of the electron excited states in the state-specific multi-reference coupled cluster theory. Hydrogen fluoride dissociation // *J. Mol. Struct.: THEOCHEM.* – 2006. – V. 768. – P. 97-101.
26. V. V. Ivanov, L. Adamowicz, and D. I. Lyakh. Dissociation of the fluorine molecule: CASCCSD method and other many-particle models // *Int. J. Quant. Chem.* – 2006. – V. 106. – P. 2875-2880.
27. D. I. Lyakh, V. V. Ivanov, L. Adamowicz. Automated generation of coupled-cluster diagrams: Implementation in the multireference state-specific coupled-cluster approach with the complete-active-space reference // *J. Chem. Phys.* – 2005. – V. 122. – ID: 024108, – P. 1-13.
28. V. V. Ivanov, D. I. Lyakh and L. Adamowicz. New indices for describing the multi-configurational nature of the coupled cluster wave function // *Mol. Phys.* – 2005. – V. 103. – No. 15-16. – P. 2131-2139.
29. V. V. Ivanov, L. Adamowicz, and D. I. Lyakh. Multireference state-specific coupled-cluster approach theory and multiconfigurationality index. BH dissociation // *Collect. Czech. Chem. Commun.* – 2005. – V. 70. – P. 1017-1033.
30. D. I. Lyakh, V. V. Ivanov, and L. Adamowicz. The coupled-cluster method with an explicit account of quadruples generated automatically // *Kharkiv University Bulletin, Chemical series. ISSN 2220-637X.* – 2003. – №596. –Issue 10(33). – P. 9 (in Russian).
31. V. V. Ivanov and D. I. Lyakh. Automated generation of coupled-cluster diagrams. Cluster expansion containing three-body clusters // *Kharkiv University Bulletin, Chemical series. ISSN 2220-637X.* – 2002. – №549. – Issue 8(31). – P. 15-20 (in Russian).

BOOK CHAPTERS

1. D. I. Lyakh, W. Joubert. Exascale Challenges in Numerical Linear and Multilinear algebras // in *Exascale Scientific Applications*, 2017, *in press*.
2. V. V. Ivanov, D. I. Lyakh, T. A. Klimenko, L. Adamowicz. Multireference State-Specific Coupled Cluster Theory with a Complete Active Space Reference // in *Practical Aspects of Computational Chemistry I: An Overview of the Last Two Decades and Current Trends*. Edited by J. Leszczynski and M. K. Shukla. Springer Science + Business Media B. V. 2012. DOI 10.1007/978-94-007-0919-5 3.
3. V. V. Ivanov, D. I. Lyakh, L. Adamowicz. Electronic excited states in the state-specific multireference coupled cluster theory with a complete-active-space reference // in “*Recent progress in coupled cluster methods: theory and applications*”. Series: “Challenges and advances in computational chemistry and physics”, Vol. 11, Cársky, Petr; Paldus, Josef; Pittner, Jiri (Eds.), Springer, 2010, P. 219-249. ISBN: 978-90-481-2884-6.

PRESENTATIONS (selected)

1. D. I. Lyakh. Efficient Electronic Structure Theory via Scale-Adaptive Coupled-Cluster Formalism // 57th Sanibel Symposium, Feb 19 – Feb 24, 2017, St. Simon’s Island, GA, USA. Book of abstracts.

Curriculum Vitae of Dmitry I. Lyakh (Liakh), Ph.D.

2. D.I. Lyakh. Linear-scaling quantum many-body theory via sparse scale-adaptive tensor algebra and massively parallel virtual processing // PACIFICHEM-2015 conference, Dec 14-20, 2015, Honolulu, HI, USA (a forthcoming talk).
3. D. I. Lyakh. ExaTensor::TAL-SH: Tensor algebra library for accelerated computing // ORNL Software Expo, Aug 5, 2015, Oak Ridge National Laboratory, Oak Ridge TN, USA.
4. D. I. Lyakh. ExaTensor: Parallel Tensor Instruction Processor // ORNL Software Expo, May 7, 2014, Oak Ridge National Laboratory, Oak Ridge TN, USA.
5. D.I. Lyakh. Sparse scale-adaptive tensor algebra for quantum many-body methods // Low-scaling and unconventional electronic structure techniques conference, Jun 2014, Telluride, CO, USA.
6. D. I. Lyakh. An efficient parallel tensor transpose algorithm for heterogeneous HPC systems based on Nvidia GPU accelerators // 54th Sanibel Symposium, Feb 16-21, 2014, St. Simon's Island, GA, USA, Book of abstracts.
7. D. I. Lyakh. Current challenges in electronic structure theory for open-shell molecules and molecular clusters // International Program at the Institute for Nuclear Theory devoted to the development of coupled-cluster methods for open-shell many-body systems, Apr 2013, University of Washington, Seattle, WA (supported by DOE).
8. D. I. Lyakh, R. J. Bartlett. An examination of the disconnected nature of Lagrange equations in the linear-scaling coupled-cluster framework // International Congress in Quantum Chemistry, Jun 25-30, 2012, Boulder, CO, USA. Book of abstracts.
9. D. I. Lyakh, R. J. Bartlett. The lost and found relation between connectivity and size-extensivity // 52th Sanibel Symposium, Feb 24 – Mar 2, 2012, St. Simon's Island, GA, USA. Book of abstracts.
10. D. I. Lyakh, R. J. Bartlett. Fully adaptive coupled-cluster approach for electron correlation accounting: Resolving multireference quantum chemical problems // 242nd ACS National Meeting, Aug 25 – Sep 2, 2011, Denver, CO, USA. Book of abstracts.
11. D. I. Lyakh, R. J. Bartlett. An adaptive coupled-cluster theory // 51th Sanibel Symposium, Feb 2011, St. Simon's Island, GA, USA. Book of abstracts.
12. D. I. Lyakh, R. J. Bartlett. Efficient quantum-chemical method designing based on the ACESIII parallel platform // 50th Sanibel Symposium, Feb 24 – Mar 2, 2010, St. Simon's Island, GA, USA. Book of abstracts.
13. D. I. Lyakh, V. V. Ivanov, L. Adamowicz. Building a wavefunction within the complete-active-space coupled-cluster with singles and doubles formalism: straightforward description of quasidegeneracy // International Workshop "Atomic, Chemical and Nuclear Developments in Coupled Cluster methods", Jun 23 – Jul 25, 2008, Seattle, WA.
14. D. I. Lyakh, V. V. Ivanov, L. Adamowicz. Automated generation of the diagrams and computer code for the state-specific multireference coupled-cluster theory // 1st International symposium "Methods and Applications of Computational Chemistry", Jun 30 – Jul 1, 2005, Kharkiv, Ukraine. Book of abstracts, P. 51.
15. D. I. Lyakh, V. V. Ivanov. Analysis of the coupled-cluster correlation energy in terms of orbital contributions // The 6th Ukrainian scientific conference for undergraduate and graduate students "Contemporary Chemical Problems", May 17-18, 2005, Kyiv, Ukraine. Book of abstracts, P. 128.
16. D. I. Lyakh, V. V. Ivanov, O. M. Kalugin. Π -electronic structure and physical-chemical properties of carbon nanotubes // XVI Ukrainian conference in inorganic chemistry, 2004, Uzhgorod, Ukraine. Book of abstracts, P. 126.
17. D. I. Lyakh, V. V. Ivanov. The coupled-cluster theory with an explicit account of higher excitations // Open Ukrainian Conference for Young Scientists, 2003, Kharkiv, Ukraine. Book of abstracts, P. 70.